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MICROCOMPUTER BASED SOFTWARE FOR LATTICE PARAMETER CALCULATIONS FOR TETRAGONAL SYSTEMS

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by

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ABSTRACT

Using BASIC programming language and an Apple IIe computer, a software program entitled LP TETR has been written to calculate the unit cell lattice parameters (a and c axis) for tetragonal crystal systems. The program is simple, well formatted and easy to run. It uses angles of diffraction (retrieved from X-ray diffraction analysis) and their corresponding hkl indices as an input for data manipulations. The output from the computer is printed out in a tabular form giving values for the 2-theta, d-spacing, hkl indices, lattice parameters ("a" and "c" values) and the Nelson-Riley function for each X-ray diffraction peak.

The program uses a linear regression analysis to obtain refined "a" and "c" values. These refined cell parameters along with the calculated unit cell volume are also printed out at the bottom of the table. The program offers the choice of printing the data on either an Apple dot matrix or Fujitsu DX2100 printer. A detailed description of the program, complete program listings and the sample lattice parameter calculations (for $PbTiO_3$ and a modified $PbTiO_3$ composition) are included.

Keywords: Lattice Parameters, Tetragonal System, X-ray Diffraction, Microcomputer, Software

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LOGICIEL DE MICRO-ORDINATEUR PERMETTANT DE CALCULER LES PARAMÈTRES DE RÉSEAU DE SYSTÈMES TÉTRAGONAUX

par

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RÉSUMÉ

Un logiciel intitulé LP TETR a été composé en langage BASIC au moyen d'un ordinateur Applie IIe; il permet de calculer les paramètres de réseau (a et c) de la maille de systèmes cristallins tétragonaux. Le programme est simple, bien composé et facile à exécuter. Les données d'entrée à manipuler sont les angles de diffraction (obtenus par diffraction des rayons X) et les indices hkl correspondants. Les résultats du traitement sont imprimés sous forme de tableau donnant les valeurs 2 thêta, l'espacement d, les indices hkl, les paramètres de réseau (a et c) et la fonction de Nelson-Riley pour chaque pic de diffraction des rayons X.

Le programme fonctionne par analyse à régression linéaire de façon à donner des valeurs plus fines de "a" et de "c". Les paramètres ainsi obtenus de même que le volume calculé de la maille sont aussi imprimés au bas du tableau. Le programme permet aussi de choisir entre l'impression des données par points ou sur imprimante modèle DX2100 de Fujitsu. Une description détaillée du programme, une impression complète du programme et le calcul des paramètres de réseau d'un échantillon ($PbTiO_3$ et $PbTiO_3$ à composition modifiée) sont inclus.

Mots clés: paramètres de réseau, système tétragonal, diffraction des rayons X, micro-ordinateur, logiciel

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INTRODUCTION

The electrical, mechanical and optical properties of solids are known to be dependent upon the crystal symmetry and the unit cell parameters. A knowledge of the unit cell parameters is therefore invaluable in the development of new materials for device applications. For example, in the development of ceramics, the density of the material is a parameter of great importance, as its mechanical, electrical and optical properties are strongly influenced by the density. Determination of the unit cell parameters is essential in determining the theoretical density of the proposed formulation. Through X-ray diffraction analysis, a pattern of interference planes can be determined which is unique to that formulation and which, if properly interpreted, can be useful in defining the unit cell.

A tetragonal unit cell is shaped like a rectangular box having two sides of equal length. Due to the symmetry of the cell we need to define only two cell parameters (i.e., "a" and "c"). The parameter "a" is the length in Angstroms of either of the two equal sides and "c" is the length in Angstroms of the third side. The reason for developing a software program for lattice parameter calculations for this system is because of our interest in $PbTiO_3$-based ceramics. $PbTiO_3$ is a piezoelectric material that belongs to the tetragonal crystal symmetry system. The high anisotropy in the crystal structure (c/a = 1.065) of $PbTiO_3$ is very advantageous as it results in a large anisotropy in the electromechanical coupling coefficients (i.e., large thickness-mode coupling coefficient (kt) to planar-mode coupling coefficient (kp) ratio). The large kt/kp coupled with a low dielectric constant of $PbTiO_3$ makes it a promising candidate for high frequency NDT transducers. Unfortunately, the large anisotropy in crystal structure of $PbTiO_3$ results in crystal strain and the development of micro/macro cracks during cooling through the Curie temperature after the sintering process. This leads to the disintegration of the material if uncontrolled grain growth is allowed to occur (1). Doping of $PbTiO_3$ by alkaline earths, rare earths and transition metal oxides reduces the c/a ratio, yielding a crack-free material (2-4).

The tetragonality (c/a ratio) in lead titanate is sensitive to both the concentration and the nature of the dopants. A large reduction in c/a ratio can adversely affect the electromechanical properties rendering it

useless for any practical application. A careful control of the amount and type of dopants as well as the processing conditions is necessary in producing the material having desired characteristics.

In the Ceramic Section at CANMET we are in the process of developing a variety of $PbTiO_3$-based compositions for high-frequency NDT transducer applications. The influence of dopants, powder-processing methods and sintering conditions on the crystal structure, microstructure and dielectric and piezoelectric properties are being investigated. As a part of this program, lattice parameters for a large number of calcined and sintered $PbTiO_3$-based compositions are being evaluated on a routine basis. A Rigaku X-ray diffractometer with CuK_α radiation and a graphite monochromator is used to record X-ray diffraction patterns for the compositions. With the help of the reference card for $PbTiO_3$ found in the "Powder Diffraction File", hkl indices are assigned to the 2-theta values retrieved from the X-ray diffraction analysis. With this information, lattice parameters of the unit cell may be calculated using appropriate equations (5) described in the next section. Since there may be as many as 50 peaks to process, performing these calculations with a hand calculator is a long and repetitious task. Therefore, the program LP TETR (lattice program for tetragonal systems) has been developed. This program is written in BASIC programming language for Apple IIe or Apple II^+ microcomputer. The detailed description of the program is given in the next section. Programs similar to LP TETR are being developed for the unit cell lattice parameter calculations for the Cubic, Hexagonal, Rhombohedral and Orthorhombic Crystal systems and will be the subject of a subsequent publication.

DETAILS OF THE PROGRAM

I. The Program Functions

The purpose of the LP TETR program is to calculate the lattice parameters of tetragonal systems from the information collected during X-ray diffraction analysis. The design of the program allows the user to

manipulate the data after it has already been input and stored. The seven functions to choose from are:

1. Input and file new data
2. Recall old data for correction
3. Recall old data for printout
4. Recall old data for addition
5. Recall old data for deletion
6. Recall old data for sorting and
7. Quit

1. INPUT AND FILE NEW DATA

This function allows for input of new data in the form of either 2-theta values (in degrees) and corresponding hkl indices or d-space values (in Angstroms) and corresponding hkl indices. After the calculations have been completed, the input data are displayed on the screen, a complete table of calculated values is printed and the data are filed on the data disc.

2. RECALL OLD DATA FOR CORRECTION

Occasionally, an error is made during the assigning process or while inputing the data. This function allows the user to change the hkl indices of as many peaks as is desired. Note that this function does not add or delete peaks. It merely adjusts hkl assignments. The entire file is recalled from the data disc, the corrections are input, then the data are recalculated, displayed, printed and refiled on the data disc under the same file name.

3. RECALL OLD DATA FOR PRINTOUT

This function simply recalls the chosen file from the data disc, displays it, then prints it. The file remains unchanged.

4. RECALL OLD DATA FOR ADDITION

This function allows for the addition of peaks to an existing data file. The addition is made to the end of the file and it is therefore recommended that the SORT function be used after the addition is complete. The

file is recalled from the data disc and the additions are input. The data are then recalculated, displayed, printed and filed on the data disc under the same file name.

5. RECALL OLD DATA FOR DELETION

If data peaks appear to be incorrect, they may be recalled from the data disc and deleted using this function. The desired peaks are deleted and the old file is compressed into a smaller one. Each time this function is used it is accompanied by a screen display, a printout and a refiling of the condensed data under the same file name.

6. RECALL OLD DATA FOR SORTING

This function sorts peaks into a file containing increasing values of 2-theta, which is the ideal situation for maximizing the accuracy of the calculated data. The file to be sorted is recalled from the data disc, sorted, recalculated, displayed, printed and refiled under the same file name.

7. QUIT

The QUIT function ends the LP TETR program.

II. The Subroutines

The LP TETR program is based on the isolation of functions into small subroutines, each of which performs a specific task. This technique greatly reduces the number of redundant lines and at the same time allows the program to be easily traced, debugged or modified. Each major subroutine begins at a new line number of a thousand (i.e., 1000, 2000, etc.) for easy reference.

1000: DATA INPUT

A general input screen asks for the date, the X-ray radiation source, the radiation wavelength (in Angstroms) and the sample identification. The user is also asked to input the data disc drive (1 or 2), the printer in use (Fujitsu or Apple Dot Matrix) and the input format (2-theta or d-space).

The peaks are input one at a time as follows, depending on the input format that was chosen:

2-theta (RETURN), h (RETURN), k (RETURN), l (RETURN)

or

d-space (RETURN), h (RETURN), k (RETURN), l (RETURN)

The screen will then skip to the next line and wait for the next set of data. When all the data have been input this routine is completed by inputing zeros for 2-theta (or d-space), h, k and l. 2-theta is required to be in units of degrees and d-space must be in Angstroms.

Should the screen fill up before all the data have been input, the data below the heading will be displaced and the data will continue to be input under the heading.

As the peaks are input, they are automatically numbered from 1 to N. A maximum of 50 peaks can be input. After this, the program will automatically continue.

2000: CALCULATIONS

The trigonometric functions in BASIC operate on theta in radians. Therefore, 2-theta (in degrees) is immediately converted to theta (in radians) using a factor of 180/Pi (57.29577951).

The d-spacing is calculated from the Bragg equation for wave interference:

$$n\lambda = 2d\sin\Theta, \text{ where } n=1$$

If the data are input using d-space format then 2-theta is calculated during the DATA INPUT routine using the Bragg equation.

The Nelson-Riley function (NRF) is a function of theta that is calculated as follows:

$$NRF = (\cos^2\Theta)/\sin\Theta + (\cos^2\Theta)/\Theta.$$

The lattice parameters of a tetragonal system are referred to as "a" and "c", where "a" is the length of one of the two equal sides of the unit cell and "c" is the length of the third side. For a tetragonal unit cell, two of the sides are of equal length, therefore the lattice parameter b is not referred to. All the interior angles of a tetragonal cell measure 90 degrees. Therefore, interior angles alpha, beta and gamma are not referred to either.

$$a = \frac{\lambda}{2} \sqrt{\frac{l_1^2 (h_2^2 + k_2^2) - l_2^2 (h_1^2 + k_1^2)}{l_1^2 \sin^2 \Theta_2 - l_2^2 \sin^2 \Theta_1}} \quad .$$

In this program, each peak is compared to the one immediately following it in the file. It is best to compare peaks with similar 2-theta values. Therefore, inputing and maintaining the peaks in increasing order of 2-theta is preferred. If one hkl assignment is incorrect, the result will be two erroneous values of "a" and "c" since it is involved in two separate calculations. The last peak in the file is not given a value of "a" since it cannot be compared with "the next peak".

$$c = \frac{\lambda . a . l}{\sqrt{4a^2 \sin^2 \Theta - \lambda^2 (h^2 + k^2)}} \quad .$$

There are certain indices which yield invalid values of "c", e.g., hko. These cases are filtered out by checking if l = 0 or if the discriminant in the denominator is negative.

Should a value of "a" or "c" be invalid, it is given the value of 0 to mark it as such.

The final part of this routine rounds off the values of "d", "a", "c" and NRF to 4 decimal places.

3000: SCREEN OUTPUT

The screen output routine displays the values of 2-theta with their hkl indices to the screen. If more than a screenful of data are to be displayed, the screen will scroll below the heading.

4000: PRINTER OUTPUT

This program is designed to produce a printout using either the Fujitsu printer or the Apple dot matrix printer.

The tombstone data are printed first, followed by the headings and the data. Each peak is numbered automatically for reference, in case correction, addition or deletion is required. Values of "a" and "c" that were marked with a zero during the calculations are omitted during printing, although they remain as zeros in the file.

The table gives each peak's corresponding a and c values so that the user can quickly identify peaks that have been assigned incorrect hkl indices.

Below the table, the refined values of "a" and "c" that correspond to the sample in question are printed out as well as the unit cell volume. "a" and "c" are calculated using the LINEAR REGRESSION ANALYSIS subroutine.

5000: LINEAR REGRESSION ANALYSIS

The refining method used to determine "a" and "c" for the sample employs the so-called "Nelson-Riley" function. Where Δa is the error involved during the measurement of "a", Nelson and Riley have shown (6) that $\Delta a/a$ is a highly linear function of $(\cos^2\Theta)/\sin\Theta + (\cos^2\Theta)/\Theta$ down to very low values. If the plots of "a" versus NRF and "c" versus NRF are extrapolated down to NRF = 0, refined values of "a" and "c" will be found with a precision as high as one part in 100,000.

To achieve this extrapolation, linear regression analysis is performed on the arrays A(*) and NRF(*), and then C(*) and NRF(*), with NRF(*) representing the "x-axis". The subsequent "y-intercepts" are the refined values of "a" and "c".

This subroutine is performed immediately following the CALCULATIONS routine. The arrays A(*), C(*) and NRF(*) are processed and the refined

values AI and CI are found. The array indices of A(*) and C(*) which were assigned zero values are overlooked in this routine.

6000: DATA CORRECTION

This routine is a simple modification of the DATA INPUT routine. The user is asked to input the numbers corresponding to the peaks which are to be corrected. After the user has input "0" to indicate that the last number has been entered, the program asks for the corrections using the same screen that is used for the DATA INPUT routine, with the chosen peak numbers automatically displayed on the left hand side of the screen.

The numbers of the peaks to be corrected are stored in an array CH(*). The numbers in this array then become the indices of TWOTH(*), H(*), K(*) and L(*). The corrected data are thus written overtop of the old data without having to manipulate the whole file. The program will not accept a value for CH(*) that is less than zero or greater than N (the total number of peaks).

7000: PRINT TO FILE

The file to be stored on the data disc is automatically assigned a file name by the program. This file name consists of the prefix LAT TETR followed by the sample identification name that was input by the user during the DATA INPUT routine. For example, if a sample was identified by the name T1, then the filename would be LAT TETR T1. Once named, the file would be stored on the disc in the drive designated during the DATA INPUT as the data disc drive.

The first few entries into the file are the tombstone data as well as the number of peaks in the file (N). Then for each of the N peaks, the following values are written to the file:

TWOTH(*),H(*),K(*),L(*),D4(*),A4(*),C4(*) and N4(*)

D4, A4, C4 and N4 represent "d", "a", "c" and the Nelson-Riley function (NRF) rounded off to four decimal places. The final two entries into the file are AI and CI which are the refined values of "a" and "c" for the sample.

8000: READ FROM FILE

This routine requires the user to input the number of the disc drive which contains the data disc (1 or 2). The program then catalogs the disc in the chosen drive and asks the user to input the name of the file to be retrieved. The user is reminded that all valid files begin with the prefix LAT TETR. The desired data are then recalled in the same order in which it was filed so that the data are input into the correct variables.

9000: MENU

The menu displays the options available to the user and asks the user to choose a function by typing the appropriate number. It is this chosen number that ultimately determines which of the sub-routines will be executed, and in which order, to perform the desired operation. After a function is complete, the program automatically returns to the menu to await further instructions.

10000: ADD DATA

Like the DATA CORRECTION routine, the ADD DATA routine is based on DATA INPUT. The new data, however, is appended to the end of the existing file. This is accomplished by numbering the peaks from N+1 onwards. After the user has entered zeros to indicate that there are no more data, N takes on the number of peaks in the new file, including the additional peaks.

If more than a screenful of additional peaks are entered, the area below the heading will be displayed so the rest of the data may be input.

11000: DELETE DATA

This routine is divided into three sections for simplicity. First, the user is asked to input the numbers corresponding to the peaks that are to be deleted. The user inputs the number zero to indicate that all the numbers have been entered. These numbers are stored in an array OM(*), which will not accept values less than zero or greater than N (the number of peaks).

Once the program knows which peaks to delete, the chosen peaks are "marked" so that they may be distinguished from the peaks that are not to be deleted. This is done by assigning the value of zero to TWOTH(*) for each of the chosen peaks.

The actual deletions are accomplished using two nested FOR..NEXT loops. The logic behind the procedure is that if TWOTH(*) is marked with a zero, then the index of all the peaks following it is decreased by one.

12000: SORT

This routine sorts the peaks in the order of increasing values of 2-theta (decreasing order of d-spacing), which is the preferred situation when calculating the lattice parameters.

Although the values of 2-theta are compared, only the indices are manipulated during this sort. Once the sort is complete, the rest of the data is rearranged accordingly. This greatly reduces the amount of time required to complete the sorting of large files.

The basic idea behind this sort is to find the smallest value of 2-theta, note the current index of the peak, then find the next smallest value of 2-theta. This calls for the use of the variables SMALL and OLDSMALL. The index of the peak with the smallest value of 2-theta is stored in the first position of array IND(*), and so on until all the indices have been put into IND(*).

To begin the sort, OLDSMALL=0 and SMALL=TWOTH(1). The TWOTH(*) values are searched from 1 to N and if at any time one of these values is smaller than SMALL, it becomes SMALL and the index of that value is noted. After one pass, SMALL contains the smallest value of 2-theta in the file and the index is put into IND(1). OLDSMALL is then assigned the value of SMALL and the process continues. It is important to make sure that SMALL is always greater than or equal to OLDSMALL, otherwise the entire array IND(*) will contain the index of the smallest value of 2-theta.

For the special case of the same 2-theta value having been assigned two or more different hkl values, the sort becomes tricky. If this happens, OLDSMALL will equal SMALL at some point in the sort and the array IND(*) must be checked to see if that peak has already been entered. If it hasn't, then the sort is continued and that value becomes SMALL. If that value has already been used, then it is skipped and the sort continues.

If the sort functions properly, then array IND(*) will contain the numbers 1 through N with no duplications and no omissions. The order of the numbers will reflect the peaks having values of 2-theta running from smallest

to largest. Once this is accomplished, temporary arrays for TWOTH(*), H(*), K(*) and L(*) are set up. Using the ordered indices stored in IND(*), values of TWOTH, H, K and L are transferred from the unsorted array into the temporary array in the sorted order. The temporary array is then transferred back to the original array but the values are now sorted in increasing order of 2-theta.

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APPENDIX I - LIST OF VARIABLES

A - ARRAY VARIABLES

All of the arrays in this program are dimensioned to 50 to account for 50 possible data peaks. Enclosed in the brackets are the subroutines containing the arrays.

A(*), C(*)	:	Lattice parameters "a" and "c" calculated for each peak. [2000, 5000]
CH(*)	:	The numbers corresponding to the peaks which are to be corrected. [6000]
D(*)	:	The distance between interference planes for each peak. [2000]
H(*), K(*), L(*)	:	The hkl indices for each peak. [all except 5000 and 9000]
HT(*), KT(*), LT(*)	:	Temporary arrays for hkl indices. [12000]
IND(*)	:	The array containing the sorted indices of the peaks. [12000]
NRF(*)	:	The Nelson-Riley function value for each peak. [2000, 5000]
CM(*)	:	The numbers corresponding to the peaks which are to be deleted. [11000]
TEMP(*)	:	A temporary array of 2-theta values. [12000]
TH(*)	:	Theta values for each peak. [2000]
TWOTH(*)	:	2-theta values for each of the peaks. [all except 5000 and 9000]
A4(*), C4(*), D4(*) N4(*)	:	Values of "a", "c", "d" and "NRF" rounded off to four decimal places. [2000, 4000, 7000, 8000]

B - STRING VARIABLES

a$: Temporary constant
D$: Control-D (CHR$(4))
DR$: Data disc drive
DTE$: Date
F$: File name
FD$: File name plus disc drive
ID$: Sample identification
RS$: Radiation source
T$: Tab for printer (CHR$(9))

C - REGULAR VARIABLES

A7AVG : Average value of "a"
A8SSNA : Sum of the products (A(i)-A7AVG)*(C(i)-C7AVG) for all i.
AB1 : Slope of "a" vs NRF
AI : Refined value of lattice parameter "a"
ASUM : Sum of A(i) for all i
C : Local constant
C7AVG : Average value of "c"
C8SSNC : Sum of the products (C(i)-C7AVG)*(NRF(i)-N7AVG) for all i.
CB1 : Slope of "c" vs NRF
CI : Refined value of lattice parameter "c"
CSUM : Sum of C(i) for all i
DEN : Denominator (local)
F : Input format type
FX : The function number which is chosen from the menu and which subsequently drives the program
HALFY : Half the radiation wavelength (Y)
I, J, JJ: Counters
M : Number of peaks to be corrected or deleted
N : Total Number of peaks in the file
N7AVG : Average value of NRF
N8SSNN : Sum of the squares of the differences between NRF(i) and N7AVG
NASUM : Sum of NRF(i)*A(i) for all i
NCSUM : Sum of NRF(i)*C(i) for all i

NNSUM : Sum of NRF(i)*NRF(i) for all i
NSUM : Sum of NRF(i) for all i
NUM : Numerator (local)
OLDSMALL: Previous value of SMALL
P : Printer type
PI : 3.141592654
Q : Flag noting if an index has already been sorted or not
SMALL : Current "small" value of 2-theta
Y : Radiation wavelength (Angstroms)
Z : Row counter for screen display

D - THE ARCSIN FUNCTION

It was necessary to define the arcsin function ASN(X) because it does not exist in APPLE BASIC. The built-in APPLE BASIC function for the arctan was used.

```
ASN(X) = ATN (X/SQR(1 - X^2))
```

APPENDIX II - SAMPLE OF OUTPUT

LATTICE PARAMETERS FOR TETRAGONAL SYSTEMS

Radiation Source : CU K ALPHA
Radiation Wavelength : 1.5405 Angstroms
Sample ID : LEAD TITANATE

Date : SEP 21 1988

	2-THETA	D-SPACE	h	k	l	'a'	'c'	NRF
1	21.393	4.1499	0	0	1	3.8999	4.1499	10.3741
2	22.782	3.8999	1	0	0	3.8999		9.6994
3	31.45	2.842	1	0	1	3.9004	4.1496	6.7947
4	32.434	2.758	1	1	0	3.9004		6.5589
5	39.185	2.297	1	1	1	3.8996	4.152	5.2424
6	43.558	2.076	0	0	2	3.9	4.152	4.5928
7	46.532	1.95	2	0	0	3.9		4.215
8	49.696	1.833	1	0	2	3.8996	4.1534	3.8582
9	51.749	1.765	2	0	1	3.8997	4.153	3.6477
10	52.419	1.744	2	1	0	3.8997		3.5822
11	55.361	1.6581	1	1	2	3.8987	4.1509	3.3113
12	57.261	1.6075	2	1	1	3.8982	4.1541	3.1496
13	65.631	1.4213	2	0	2	3.8996	4.1523	2.5365
14	67.628	1.3841	0	0	3	3.8995	4.1523	2.4101
15	67.929	1.3787	2	2	0	3.8995		2.3917
16	70.469	1.3351	2	1	2	3.8984	4.1522	2.2413
17	72.148	1.3081	2	2	1	3.8983	4.1529	2.147
18	72.379	1.3045	1	0	3	3.9	4.1527	2.1344
19	72.669	1.3	3	0	0	3.9		2.1186
20	76.781	1.2403	3	0	1	3.8989	4.1524	1.9061
21	77.024	1.237	1	1	3	3.9001	4.1521	1.8942
22	77.297	1.2333	3	1	0	3.9001		1.8809
23	81.341	1.1819	3	1	1	3.8987	4.1528	1.6932
24	84.245	1.1484	2	2	2	3.8985	4.1532	1.5685
25	86.066	1.1287	2	0	3	3.8986	4.1532	1.4943
26	88.727	1.1016	3	0	2	3.8988	4.1525	1.3911
27	90.551	1.0841	2	1	3	3.8997	4.1519	1.3236
28	90.819	1.0816	3	2	0	3.8997		1.3139
29	93.201	1.0601	3	1	2	3.8991	4.1517	1.2302
30	94.788	1.0465	3	2	1	3.899	4.1532	1.1766
31	95.776	1.0383	0	0	4	3.8852	4.1532	1.1442
32	100.326	1.0031	1	0	4	3.8981	4.1522	1.0032
33	104.129	.9766	2	2	3	3.8988	4.1515	.8951
34	104.416	.9747	4	0	0	3.8988		.8873
35	104.905	.9715	1	1	4	3.9002	4.1521	.8741
36	106.821	.9593	3	2	2	3.8995	4.1547	.8237
37	108.497	.9491	4	0	1	3.8996	4.153	.7812
38	108.749	.9476	3	0	3	3.8992	4.1535	.7749
39	109.071	.9457	4	1	0	3.8992		.767
40	113.28	.9222	4	1	1			

a = 3.89838929
c = 4.15322057

Cell Volume = 63.1183166

LATTICE PARAMETERS FOR TETRAGONAL SYSTEMS

Radiation Source : Cu Date : 2/9/87
Radiation Wavelength : 1.5406 Angstroms
Sample ID : $(Pb,Ca)TiO_3$ - $Pb(Co,W)O_3$

	2-THETA	D-SPACE	h	k	l	'a'	'c'	NRF
1	21.9	4.0552	0	0	1	3.8971	4.0552	10.1182
2	22.8	3.8971	1	0	0	3.8971		9.6912
3	31.85	2.8074	1	0	1	3.8872	4.059	6.6972
4	32.55	2.7486	1	1	0	3.8872		6.532
5	39.55	2.2768	1	1	1	3.8946	4.0471	5.1831
6	44.75	2.0236	0	0	2	3.8949	4.0471	4.4359
7	46.6	1.9474	2	0	0	3.8949		4.2069
8	50.8	1.7958	1	0	2	3.8847	4.0505	3.7431
9	56.4	1.6301	1	1	2	3.8921	4.0463	3.2217
10	57.6	1.5989	2	1	1	3.8915	4.0501	3.1217
11	66.6	1.403	2	0	2	3.8912	4.0504	2.4744
12	68.1	1.3757	2	2	0	3.8912		2.3812
13	69.65	1.3489	0	0	3	3.8907	4.0466	2.2887
14	71.45	1.3192	2	1	2	3.8828	4.0578	2.1858
15	72.65	1.3004	2	2	1	3.8841	4.0461	2.1196
16	74.4	1.2741	1	0	3	3.8849	4.046	2.0266
17	77.3	1.2333	3	0	1	3.8845	4.0503	1.8807
18	78.95	1.2117	1	1	3	3.8925	4.0483	1.802
19	81.7	1.1777	3	1	1	3.8926	4.0475	1.6773
20	85.2	1.138	2	2	2	3.8939	4.0446	1.5293
21	88.05	1.1084	2	0	3	3.8933	4.0449	1.4168
22	89.7	1.0922	3	0	2	3.8873	4.0601	1.3548
23	91.2	1.0781	3	2	0	3.8873		1.3002
24	92.5	1.0664	2	1	3	3.8918	4.0478	1.2544
25	94.2	1.0515	3	1	2	3.8906	4.0511	1.1963
26	95.25	1.0427	3	2	1	3.8907	4.05	1.1614
27	103.65	.9799	1	0	4	3.8929	4.0499	.9083
28	104.65	.9732	4	0	0	3.8929		.881
29	106.15	.9636	2	2	3	3.8849	4.0563	.8411
30	108.1	.9515	3	2	2	3.8869	4.0492	.7911
31	111	.9347	3	0	3	3.8909	4.0447	.7205
32	113.9	.919	4	1	1	3.8908	4.0471	.6541
33	115.85	.9091	3	1	3	3.8833	4.0564	.6117
34	117.95	.8989	2	0	4	3.8961	4.0528	.5681
35	118.65	.8956	3	3	1	3.896	4.0555	.554
36	123.05	.8763	2	1	4	3.8944	4.0561	.4703
37	124.4	.8708	4	2	0	3.8944		.4463
38	128.3	.8559	4	1	2	3.8932	4.0545	.381
39	129.65	.8511	4	2	1			

a = 3.88983415 Cell Volume = 61.2817806

APPENDIX III - PROGRAM LISTING

```
10  REM      LP TETR
11 :
12  REM      ************************************************
13  REM      *  Lattice parameters for tetragonal systems  *
16  REM      ************************************************
17 :
18 :
19 :
20 :
400  DIM TWOTH(50)
401  DIM H(50)
402  DIM K(50)
403  DIM L(50)
404  DIM TH(50)
405  DIM D(50)
406  DIM NRF(50)
407  DIM A(50)
408  DIM C(50)
409  DIM D4(50)
410  DIM A4(50)
411  DIM C4(50)
412  DIM N4(50)
413  DIM CH(20)
414  DIM OM(50)
415  DIM IND(50)
416  DIM TEMP(50)
417  DIM HT(50)
418  DIM KT(50)
419  DIM LT(50)
440 :
441 PI = 3.141592654
442  DEF  FN ASN(X) =  ATN (X /  SQR (1 - X ^ 2)) * 180 / PI
480 :
481 :
482 :
483  REM          --------------------
484  REM             DRIVER PROGRAM
485  REM          --------------------
486 :
487 :
500  GOSUB 9000
510  ON FX GOSUB 600,700,800,850,865,890,970
520  GOTO 500
600 :
601  REM          1.  input and file new data
602 :
603 :
610  GOSUB 1000
620  GOSUB 2000
630  GOSUB 5000
640  GOSUB 3000
650  GOSUB 4000
```

```
660  GOSUB 7000
670  RETURN
700 :
701  REM          2.  recall old data for correction
702 :
703 :
710  GOSUB 8000
720  GOSUB 6000
730  GOSUB 2000
740  GOSUB 5000
750  GOSUB 3000
760  GOSUB 4000
770  GOSUB 7000
780  RETURN
800 :
801  REM          3.  recall old data for printout
802 :
803 :
810  GOSUB 8000
820  GOSUB 3000
830  GOSUB 4000
840  RETURN
850 :
852  REM          4.  recall old data and add to it
853 :
854 :
855  GOSUB 8000
857  GOSUB 10000
858  GOSUB 2000
859  GOSUB 5000
860  GOSUB 3000
861  GOSUB 4000
862  GOSUB 7000
863  RETURN
865 :
866  REM          5.  recall old data and omit selected data
867 :
868 :
869  GOSUB 8000
870  GOSUB 11000
871  GOSUB 2000
872  GOSUB 5000
873  GOSUB 3000
874  GOSUB 4000
875  GOSUB 7000
880  RETURN
890 :
891  REM              6.  recall data and sort
892 :
893 :
895  GOSUB 8000
897  GOSUB 12000
900  GOSUB 2000
902  GOSUB 5000
904  GOSUB 3000
906  GOSUB 4000
908  GOSUB 7000
910  RETURN
970 :
971  REM              7.  quit
```

```
972 :
973 :
974  HOME
975  END
980 :
981 :
982 :
983  REM           --------------------
984  REM              LIST PROGRAM
985  REM           --------------------
986 :
987 :
988  HOME : VTAB 12
989  PRINT "Type of printer : 1. Apple Dot Matrix"
990  PRINT "                  2. Fujitsu         ";: INPUT " ";P
991  IF P < > 1 AND P < > 2 THEN  VTAB 12: GOTO 989
992  GOSUB 4910
994  IF P = 1 THEN  PRINT  CHR$ (27) CHR$ (76)"010": REM  Set margin for Apple Dot
995  IF P = 2 THEN  PRINT  CHR$ (27)"1" CHR$ (10): REM  Set margin for Fujitsu
997  LIST
998  PRINT  CHR$ (4);"PR#3"
999  END
1000 :
1010 :
1020 :
1021  REM           --------------------
1022  REM               DATA INPUT
1023  REM           --------------------
1030 :
1040  REM           general input
1041 :
1042 :
1045  HOME
1046  PRINT : PRINT
1050  PRINT  TAB( 5);"LATTICE PARAMETERS FOR "
1051  PRINT  TAB( 09);"TETRAGONAL SYSTEMS"
1059  PRINT : PRINT
1060  PRINT "Input the following (no commas) :"
1065  PRINT
1070  PRINT  TAB( 07);"Todays date :";: INPUT " ";DTE$
1080  PRINT  TAB( 07);"Radiation Source :";: INPUT " ";RS$
1090  PRINT  TAB( 07);"Radiation Wavelength :";: INPUT " ";Y
1100  PRINT  TAB( 07);"Sample ID :";: INPUT " ";ID$
1110  PRINT  TAB( 07);"Data disc drive :";: INPUT " ";DR$
1120  IF DR$ < > "1" AND DR$ < > "2" THEN  VTAB 13: GOTO 1110
1124  PRINT  TAB( 07);"Type of printer:  1. Apple Dot Matrix"
1125  PRINT  TAB( 07);"                  2. Fujitsu         ";: INPUT " ";P
1126  IF P < > 1 AND P < > 2 THEN  VTAB 14: GOTO 1124
1127  GOSUB 1900
1130 HALFY = Y / 2
1135  ON F GOSUB 1140,1340
1137  RETURN
1140 :
1141  REM            input of 2-theta and hkl values
1142 :
1143 :
1145  HOME
1147  POKE 34,8
1150  PRINT : PRINT
1160  PRINT "Input 2-theta values and corresponding hkl values"
```

```
1180  PRINT "(Input zeros to end file)"
1190  PRINT : PRINT
1200  PRINT "#    2-THETA          H      K      L"
1210  PRINT "-------------------------------------"
1225 Z = 9
1230 I = 1
1235  IF Z > 22 THEN  HOME :Z = 9
1236  IF I > 50 THEN  GOTO 1290
1238  HTAB 1: VTAB Z: PRINT I
1240  HTAB 6: VTAB Z: INPUT " ";TWOTH(I)
1245  IF TWOTH(I) < 0 THEN 1240
1250  HTAB 22: VTAB Z: INPUT " ";H(I)
1260  HTAB 29: VTAB Z: INPUT " ";K(I)
1270  HTAB 36: VTAB Z: INPUT " ";L(I)
1279  PRINT : PRINT
1282 Z = Z + 1
1285  IF TWOTH(I) <  > 0 THEN I = I + 1: GOTO 1235
1290 N = I - 1
1295  POKE 34,0
1300  RETURN
1340 :
1341  REM              input of d-space and hkl values
1342 :
1343 :
1345  HOME
1347  POKE 34,8
1350  PRINT : PRINT
1360  PRINT "Input d-space values and corresponding hkl values"
1380  PRINT "(Input zeros to end file)"
1390  PRINT : PRINT
1400  PRINT "#    D-SPACE          H      K      L"
1410  PRINT "-------------------------------------"
1425 Z = 9
1430 I = 1
1435  IF Z > 22 THEN  HOME :Z = 9
1436  IF I > 50 THEN  GOTO 1490
1438  HTAB 1: VTAB Z: PRINT I
1440  HTAB 6: VTAB Z: INPUT " ";D(I)
1445  IF D(I) < 0 THEN 1440
1447  IF D(I) <  > 0 THEN TWOTH(I) = 2 *  FN ASN(Y / 2 / D(I))
1448  IF D(I) <  > 0 THEN TWOTH(I) =  INT (TWOTH(I) * 1000 + .5) / 1000
1450  HTAB 22: VTAB Z: INPUT " ";H(I)
1460  HTAB 29: VTAB Z: INPUT " ";K(I)
1470  HTAB 36: VTAB Z: INPUT " ";L(I)
1479  PRINT : PRINT
1482 Z = Z + 1
1485  IF D(I) <  > 0 THEN I = I + 1: GOTO 1435
1490 N = I - 1
1495  POKE 34,0
1500  RETURN
1900 :
1901  REM          choice of input format
1902 :
1903 :
1905  HOME
1910  PRINT  TAB( 7);"Input format : 1. 2-theta & hkl"
1920  PRINT  TAB( 7);"               2. d-space & hkl";
1930  INPUT " ";F
1940  IF F <  > 1 AND F <  > 2 THEN 1905
1950  RETURN
```

```
2000 :
2010 :
2015 :
2020  REM          --------------------
2030  REM              CALCULATIONS
2035  REM          --------------------
2036 :
2065  REM          theta : 'd' : Nelson-Riley function
2066 :
2067 :
2068  HOME
2069  HTAB 20: VTAB 15: PRINT "Calculating ......"
2070 :
2071 :
2075  FOR I = 1 TO N
2080 TH(I) = TWOTH(I) / (2 * 57.29577951)
2090 D(I) = Y / (2 *  SIN (TH(I)))
2092 C =  COS (TH(I)) ^ 2
2095 NRF(I) = C /  SIN (TH(I)) + C / TH(I)
2100  NEXT
2105 :
2106  REM          'a'
2107 :
2108 :
2110  FOR I = 1 TO N - 1
2120 NUM = L(I) ^ 2 * (H(I + 1) ^ 2 + K(I + 1) ^ 2) - L(I + 1) ^ 2 * (H(I) ^ 2 + K(I) ^ 2)
2130 DEN = L(I) ^ 2 *  SIN (TH(I + 1)) ^ 2 - L(I + 1) ^ 2 *  SIN (TH(I)) ^ 2
2135  IF DEN = 0 THEN A(I) = 0: GOTO 2150
2140 A(I) = HALFY *  SQR (NUM / DEN)
2150  NEXT
2160 :
2170  REM          'c'
2180 :
2181 :
2190 I = 0
2200 I = I + 1
2210  IF I > N THEN 2270
2220  IF L(I) = 0 THEN C(I) = 0: GOTO 2200
2240 C = 4 * A(I) ^ 2 *  SIN (TH(I)) ^ 2 - Y ^ 2 * (H(I) ^ 2 + K(I) ^ 2)
2245  IF C <  = 0 THEN C(I) = 0: GOTO 2260
2247 DEN =  SQR (C)
2248 NUM = Y * A(I) * L(I)
2250 C(I) = NUM / DEN
2260  GOTO 2200
2263 :
2264  REM          rounding off to 4 decimal places the
2265  REM            values of 'd', 'a', 'c', and the
2266  REM            Nelson-Riley function
2267 :
2268 :
2270  FOR I = 1 TO N
2275 D4(I) =  INT (D(I) * 10000 + .5) / 10000
2280 A4(I) =  INT (A(I) * 10000 + .5) / 10000
2290 C4(I) =  INT (C(I) * 10000 + .5) / 10000
2300 N4(I) =  INT (NRF(I) * 10000 + .5) / 10000
2310  NEXT
2320  RETURN
3000 :
3010 :
3015 :
```

```
3020  REM          --------------------
3021  REM            SCREEN OUTPUT
3022  REM          --------------------
3030 :
3040  REM           outputs to the screen values of 2-theta,
3041  REM             h,k and l for verification
3060 :
3061 :
3065  HOME
3066  POKE 34,4
3070  PRINT : PRINT
3075  PRINT "#    2-THETA         H     K     L"
3076  PRINT "-------------------------------------"
3080  FOR I = 1 TO N
3085  PRINT I;
3090  HTAB 7: PRINT TWOTH(I);
3092  HTAB 23: PRINT H(I);
3093  HTAB 30: PRINT K(I);
3094  HTAB 37: PRINT L(I)
3120  NEXT
3125  POKE 34,0
3200  RETURN
4000 :
4005 :
4010 :
4020  REM          --------------------
4021  REM            PRINTER OUTPUT
4022  REM          --------------------
4023 :
4024  REM           tables the values of 2-theta, 'd', 'a',
4025  REM            'c', hkl, and the Nelson-Riley function
4026 :
4027 :
4540  REM          sets up printer of choice
4545 :
4546 :
4550  GOSUB 4910
4559 :
4560  REM           title block
4561 :
4562 :
4565  PRINT : PRINT
4566  PRINT T$"LATTICE PARAMETERS FOR TETRAGONAL SYSTEMS"
4567  PRINT
4568  PRINT T$"Radiation Source : ";RS$;T$;T$;T$;T$;T$;T$;"Date : ";DTE$
4569  PRINT T$"Radiation Wavelength : ";Y;" Angstroms"
4570  PRINT T$"Sample ID : ";ID$
4571 :
4572  REM          table of values
4573 :
4574 :
4575  PRINT : PRINT : PRINT T$;
4576  FOR I = 1 TO 100
4577  PRINT "-";
4578  NEXT
4579  PRINT
4580  PRINT T$T$;"2-THETA";T$;"D-SPACE";
4585  PRINT T$;"h";T$;"k";T$;"l";T$;"'a'";T$;"'c'";T$;"NRF"
4587  PRINT T$;
4590  FOR I = 1 TO 100
```

```
4592  PRINT "-";
4593  NEXT
4594  PRINT
4600  FOR I = 1 TO N
4610  PRINT T$I;T$;TWOTH(I);T$;D4(I);T$;H(I);T$;K(I);T$;L(I);
4613  IF A4(I) = 0 THEN  PRINT T$;" ";: GOTO 4620
4615  PRINT T$;A4(I);
4620  IF C4(I) = 0 THEN  PRINT T$;" ";: GOTO 4635
4630  PRINT T$;C4(I);
4635  IF I = N THEN  PRINT T$;" ": GOTO 4650
4640  PRINT T$;N4(I)
4650  NEXT
4660  PRINT T$;
4670  FOR I = 1 TO 100
4680  PRINT "-";
4690  NEXT
4695  PRINT
4700  PRINT : PRINT : PRINT
4710  PRINT T$T$;"a = ";AI;T$T$;"           Cell Volume = ";AI * AI * CI
4720  PRINT T$T$;"c = ";CI
4800  PRINT  CHR$ (4);"PR#3"
4900  RETURN
4910 :
4911  REM          printer commands and tabbing
4912 :
4913 :
4920  ON P GOSUB 4930,4960
4921  RETURN
4930 :
4931 :
4934  REM            Apple Dot Matrix printer
4935 :
4936  PRINT  CHR$ (4);"PR#1"
4937  PRINT  CHR$ (27) CHR$ (81): PRINT  CHR$ (9);"132N"
4938  PRINT  CHR$ (9); CHR$ (1)
4939  PRINT  CHR$ (27) CHR$ (48): PRINT  CHR$ (27) CHR$ (76)"1"
4940  PRINT  CHR$ (27) CHR$ (40)"015,025,041,057,063,069,075,091,107."
4941 T$ =  CHR$ (9)
4950  RETURN
4960 :
4961 :
4962 : REM          Fujitsu printer
4963 :
4964 :
4966  PRINT  CHR$ (4);"PR#1"
4967  PRINT  CHR$ (27) CHR$ (15)
4968  PRINT  CHR$ (9)"142N"
4969  PRINT  CHR$ (27)"N" CHR$ (6): PRINT  CHR$ (27)"1" CHR$ (1)
4970  PRINT  CHR$ (27) CHR$ (73)
4972  PRINT  CHR$ (27) CHR$ (68) CHR$ (15) CHR$ (25) CHR$ (41) CHR$ (57) CHR$ (63) CHR$ (69) CHR$ (75) CHR$ (91) CHR$ (107) CHR
$ (0)
4974 T$ =  CHR$ (9)
4976  PRINT T$" ";
4980  RETURN
5000 :
5010 :
5020 :
5030  REM          -------------------------------
5031  REM            LINEAR REGRESSION ANALYSIS
5032  REM          -------------------------------
```

```
5050 :
5060  REM          'a' parameter vs Nelson-Riley function
5065 :
5070 :
5080 NASUM = 0:NNSUM = 0:NSUM = 0:ASUM = 0
5085 J = 0
5090  FOR I = 1 TO N - 1
5095  IF A(I) = 0 THEN 5140
5100 NASUM = NASUM + NRF(I) * A(I)
5110 NNSUM = NNSUM + NRF(I) ^ 2
5120 NSUM = NSUM + NRF(I)
5130 ASUM = ASUM + A(I)
5135 J = J + 1
5140  NEXT
5150 N7AV6 = NSUM / J
5160 A7AV6 = ASUM / J
5170 N8SSNN = NNSUM - NSUM ^ 2 / J
5180 A8SSNA = NASUM - NSUM * ASUM / J
5190 AB1 = A8SSNA / N8SSNN
5200 AI = A7AV6 - AB1 * N7AV6
5500 :
5510 :
5520  REM          'c' parameter vs Nelson-Riley function
5530 :
5540 :
5550 NCSUM = 0:NNSUM = 0:NSUM = 0:CSUM = 0
5560 J = 0
5570  FOR I = 1 TO N - 1
5580  IF C(I) = 0 THEN 5640
5590 NCSUM = NCSUM + NRF(I) * C(I)
5600 NNSUM = NNSUM + NRF(I) ^ 2
5610 NSUM = NSUM + NRF(I)
5620 CSUM = CSUM + C(I)
5630 J = J + 1
5640  NEXT
5650 N7AV6 = NSUM / J
5660 C7AV6 = CSUM / J
5670 N8SSNN = NNSUM - NSUM ^ 2 / J
5680 C8SSNC = NCSUM - NSUM * CSUM / J
5690 CB1 = C8SSNC / N8SSNN
5700 CI = C7AV6 - CB1 * N7AV6
5800  RETURN
6000 :
6001 :
6002 :
6003  REM          --------------------
6004  REM             DATA CORRECTION
6005  REM          --------------------
6006 :
6007  REM           asks which values to correct
6008 :
6009 :
6010  HOME
6020  PRINT : PRINT
6030  PRINT "WHICH NUMBER(S) DO YOU WISH TO CORRECT ?"
6040  PRINT "   (ENTER ZERO WHEN FINISHED)"
6050  PRINT
6060 I = 1
6070  INPUT " ";CH(I)
6075  IF CH(I) < 0 OR CH(I) > N THEN 6070
```

```
6080  IF CH(I) = 0 THEN 6100
6090 I = I + 1
6095  GOTO 6070
6100 M = I - 1
6110 :
6120  REM          choice of input format
6121 :
6122 :
6130  GOSUB 1900
6140  ON F GOSUB 6200,6400
6150  RETURN
6200 :
6202  REM            input corrected data (2-theta)
6203 :
6204 :
6210  HOME
6215  POKE 34,8
6220  PRINT : PRINT
6223  PRINT "Input the corrected values of 2-theta, h, k and l"
6227  PRINT : PRINT
6230  PRINT "#    2-THETA          H      K      L"
6240  PRINT "-------------------------------------"
6245 Z = 9
6250  FOR J = 1 TO M
6260 I = CH(J)
6265  IF Z > 22 THEN  HOME :Z = 9
6270  HTAB 1: VTAB Z: PRINT I
6280  HTAB 6: VTAB Z: INPUT " ";TWOTH(I)
6290  HTAB 22: VTAB Z: INPUT " ";H(I)
6300  HTAB 29: VTAB Z: INPUT " ";K(I)
6310  HTAB 36: VTAB Z: INPUT " ";L(I)
6320  PRINT : PRINT
6325 Z = Z + 1
6330  NEXT
6335  POKE 34,0
6340  RETURN
6400 :
6402  REM            input corrected data (d-space)
6403 :
6404 :
6410  HOME
6415  POKE 34,8
6420  PRINT : PRINT
6423  PRINT "Input the corrected values of d-space, h, k and l"
6427  PRINT : PRINT
6430  PRINT "#    D-SPACE          H      K      L"
6440  PRINT "-------------------------------------"
6445 Z = 9
6450  FOR J = 1 TO M
6460 I = CH(J)
6465  IF Z > 22 THEN  HOME :Z = 9
6470  HTAB 1: VTAB Z: PRINT I
6480  HTAB 6: VTAB Z: INPUT " ";D(I)
6485  IF D(I) <  > 0 THEN TWOTH(I) = 2 *  FN ASN(Y / 2 / D(I))
6487  IF D(I) <  > 0 THEN TWOTH(I) =  INT (TWOTH(I) * 1000 + .5) / 1000
6490  HTAB 22: VTAB Z: INPUT " ";H(I)
6500  HTAB 29: VTAB Z: INPUT " ";K(I)
6510  HTAB 36: VTAB Z: INPUT " ";L(I)
6520  PRINT : PRINT
6525 Z = Z + 1
```

```
6530  NEXT
6535  POKE 34,0
6540  RETURN
7000 :
7001 :
7002 :
7003  REM          --------------------
7004  REM             PRINT TO FILE
7005  REM          --------------------
7006 :
7007  REM           prints the data to file "F$"
7008 :
7009 :
7010 D$ =  CHR$ (4)
7013 F$ = "LAT TETR " + ID$
7015 FD$ = F$ + ",D" + DR$
7020  PRINT D$;"OPEN";FD$
7030  PRINT D$;"WRITE";F$
7040  PRINT ID$: PRINT DTE$: PRINT RS$: PRINT Y: PRINT HALFY: PRINT N
7050  FOR I = 1 TO N
7060  PRINT TWOTH(I): PRINT H(I): PRINT K(I): PRINT L(I)
7063  PRINT D4(I): PRINT A4(I): PRINT C4(I): PRINT N4(I)
7070  NEXT
7075  PRINT AI: PRINT CI
7080  PRINT D$;"CLOSE";F$
7100  RETURN
8000 :
8001 :
8002 :
8003  REM          --------------------
8004  REM             READ FROM FILE
8005  REM          --------------------
8006 :
8007  REM          reads data from file "F$"
8008 :
8009 :
8010  HOME
8011  PRINT : PRINT : PRINT
8015  PRINT : PRINT
8025  INPUT "Which drive contains the data disc : ";DR$
8026  IF DR$ <  > "1" AND DR$ <  > "2" THEN  VTAB 6: GOTO 8025
8028  PRINT "Type of printer:  1. Apple Dot Matrix"
8029  PRINT "                  2. Fujitsu         ";: INPUT " ";P
8030  IF P <  > 1 AND P <  > 2 THEN  VTAB 7: GOTO 8028
8032  HOME
8033  PRINT  CHR$ (4);"CATALOG D" + DR$
8035  PRINT : PRINT
8042  PRINT "Input the name of the file you wish to input: "
8043  PRINT "(valid files are in the form 'LAT TETR ....' )"
8044  PRINT
8045  INPUT " ";F$
8050 D$ =  CHR$ (4)
8060  PRINT D$;"OPEN";F$
8070  PRINT D$;"READ";F$
8080  INPUT ID$: INPUT DTE$: INPUT RS$: INPUT Y: INPUT HALFY: INPUT N
8090  FOR I = 1 TO N
8100  INPUT TWOTH(I): INPUT H(I): INPUT K(I): INPUT L(I)
8105  INPUT D4(I): INPUT A4(I): INPUT C4(I): INPUT N4(I)
8110  NEXT
8115  INPUT AI: INPUT CI
```

```
8120  PRINT D$;"CLOSE";F$
8130  RETURN
9000 :
9001 :
9002 :
9003  REM           --------------------
9004  REM                 MENU
9005  REM           --------------------
9006 :
9007  REM           displays menu that directs program
9008 :
9009 :
9010  PRINT  CHR$ (4);"PR#3"
9515  HOME
9520  PRINT : PRINT
9530  PRINT  TAB( 5);"LATTICE PARAMETERS FOR TETRAGONAL SYSTEMS"
9540  HTAB 10: VTAB 8: PRINT "choose the number of the desired function"
9550  HTAB 20: VTAB 11: PRINT "1.  Input and file new data"
9560  HTAB 20: VTAB 13: PRINT "2.  Recall old data for correction"
9570  HTAB 20: VTAB 15: PRINT "3.  Recall old data for printout"
9575  HTAB 20: VTAB 17: PRINT "4.  Recall old data for addition"
9576  HTAB 20: VTAB 19: PRINT "5.  Recall old data for deletion"
9577  HTAB 20: VTAB 21: PRINT "6.  Recall old data for sorting"
9578  HTAB 20: VTAB 23: PRINT "7.  Quit"
9580  GET FX: PRINT
9590  IF FX < 1 OR FX > 7 THEN 9580
9600  RETURN
10000 :
10001 :
10002 :
10003  REM           --------------------
10004  REM                ADD DATA
10005  REM           --------------------
10006 :
10007  REM           adds data to an existing file
10008 :
10009 :
10015  REM           choice of input format
10016 :
10017 :
10020  GOSUB 1900
10025  ON F GOSUB 10040,10240
10030  RETURN
10031 :
10032 :
10035  REM           2-theta input
10036 :
10037 :
10040  HOME
10042  POKE 34,8
10044  PRINT : PRINT
10046  PRINT "Input 2-theta values and corresonding hkl values to be added"
10050  PRINT "        (Input zeros to finish)"
10060  PRINT : PRINT
10070  PRINT "#    2-THETA          H      K      L"
10080  PRINT "-----------------------------------"
10090 I = N + 1
10092 Z = 9
10100  IF Z > 22 THEN  HOME :Z = 9
10105  HTAB 1: VTAB Z: PRINT I
```

```
10106  HTAB 6: VTAB Z: INPUT " ";TWOTH(I)
10107  HTAB 22: VTAB Z: INPUT " ";H(I)
10108  HTAB 29: VTAB Z: INPUT " ";K(I)
10109  HTAB 36: VTAB Z: INPUT " ";L(I)
10110  PRINT : PRINT
10115  IF TWOTH(I) = 0 THEN 10140
10120 I = I + 1
10125 Z = Z + 1
10130  GOTO 10100
10140 N = I - 1
10145  POKE 34,0
10150  RETURN
10231 :
10232 :
10235  REM           d-space input
10236 :
10237 :
10240  HOME
10242  POKE 34,8
10244  PRINT : PRINT
10246  PRINT "Input d-space values and corresonding hkl values to be added"
10250  PRINT "        (Input zeros to finish)"
10260  PRINT : PRINT
10270  PRINT "#    D-SPACE          H      K      L"
10280  PRINT "-------------------------------------"
10290 I = N + 1
10292 Z = 9
10300  IF Z > 22 THEN  HOME :Z = 9
10305  HTAB 1: VTAB Z: PRINT I
10306  HTAB 6: VTAB Z: INPUT " ";D(I)
10307  HTAB 22: VTAB Z: INPUT " ";H(I)
10308  HTAB 29: VTAB Z: INPUT " ";K(I)
10309  HTAB 36: VTAB Z: INPUT " ";L(I)
10310  PRINT : PRINT
10315  IF D(I) = 0 THEN 10340
10317 TWOTH(I) = 2 *  FN ASN(Y / 2 / D(I))
10318 TWOTH(I) =  INT (TWOTH(I) * 1000 + .5) / 1000
10320 I = I + 1
10325 Z = Z + 1
10330  GOTO 10300
10340 N = I - 1
10345  POKE 34,0
10350  RETURN
11000 :
11001 :
11002 :
11003  REM          --------------------
11004  REM               DELETE DATA
11005  REM          --------------------
11006 :
11007  REM           input data number(s) to be deleted
11008 :
11009 :
11010  HOME
11020  PRINT : PRINT
11030  PRINT "Input the number(s) of the peaks to be deleted"
11040  PRINT "    (Input zero when finished)"
11050  PRINT
11060 I = 1
11070  INPUT " ";DM(I)
```

```
11080  IF OM(I) > N OR OM(I) < 0 THEN 11070
11090  IF OM(I) = 0 THEN 11120
11100 I = I + 1
11110  GOTO 11070
11120 M = I - 1
11130 :
11140  REM          'marks' the values to be deleted
11150 :
11160 :
11170  FOR I = 1 TO M
11180 C = OM(I)
11190 TWOTH(C) = 0
11200  NEXT
11210 :
11220  REM          deletes the 2-theta, h, k, and l values that
11230  REM            were chosen and condenses the remaining data
11240  REM            into a smaller array - to complete this
11250  REM            process, recalculate this file
11260 :
11270 :
11280 C = 0
11290  FOR I = 1 TO N
11300  IF TWOTH(I) <  > 0 THEN 11390
11310 C = C + 1
11320  FOR J = I TO N - C
11330 TWOTH(J) = TWOTH(J + 1)
11340 H(J) = H(J + 1)
11350 K(J) = K(J + 1)
11360 L(J) = L(J + 1)
11370  NEXT J
11380 I = I - 1
11390  NEXT I
11400 N = N - M
11410  RETURN
12000 :
12001 :
12002 :
12003  REM          --------------------
12004  REM                  SORT
12005  REM          --------------------
12010 :
12014 :
12015  HOME
12016  HTAB 20: VTAB 15: PRINT "Sorting ......"
12050 :
12055 :
12060  REM          sorts indices so indice number of smallest
12070  REM            2-theta value is first, etc.
12080 :
12090 :
12100 OLDSMALL = 0
12110  FOR I = 1 TO N
12115 J = 1
12116 SMALL = TWOTH(J):C = J
12117 :
12118  IF SMALL <  > OLDSMALL THEN 12125
12119 Q = 0
12120  FOR JJ = 1 TO I - 1
12121  IF J = IND(JJ) THEN Q = 1
12122  NEXT JJ
```

```
12123 IF Q = 0 THEN 12128
12124 :
12125  IF SMALL > OLDSMALL THEN 12128
12126 J = J + 1
12127  GOTO 12116
12128  FOR J = 1 TO N
12129 :
12130  IF TWOTH(J) <  > SMALL AND TWOTH(J) <  > OLDSMALL THEN 12143
12131 Q = 0
12132  FOR JJ = 1 TO I - 1
12133  IF J = IND(JJ) THEN Q = 1
12134  NEXT JJ
12135  IF Q = 1 THEN 12147
12136 :
12143  IF TWOTH(J) > SMALL OR TWOTH(J) < OLDSMALL THEN 12147
12145 SMALL = TWOTH(J):C = J
12147  NEXT J
12150 IND(I) = C
12155 OLDSMALL = SMALL
12160  NEXT I
12170 :
12180  REM          reassigns indices so that smallest value of
12190  REM            2-theta and corresponding hkl has indice 1, etc.
12200 :
12210 :
12220  FOR I = 1 TO N
12225 C = IND(I)
12230 TEMP(I) = TWOTH(C)
12232 HT(I) = H(C)
12233 KT(I) = K(C)
12234 LT(I) = L(C)
12240  NEXT
12250  FOR I = 1 TO N
12260 TWOTH(I) = TEMP(I)
12262 H(I) = HT(I)
12263 K(I) = KT(I)
12264 L(I) = LT(I)
12270  NEXT
12280  RETURN
```